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NEWS 21 SEP 25
                 CAS REGISTRY(SM) updated with amino acid codes for pyrrolysine
NEWS 22 SEP 25
NEWS 23 SEP 28 CEABA-VTB classification code fields reloaded with new
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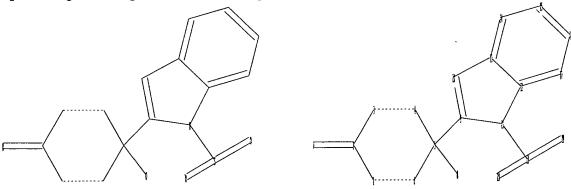
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1 2 3 4 5 6 9 10 11 12 13 14 15 16 17

chain bonds :

2-7 5-8 5-9 13-18 18-19 18-20

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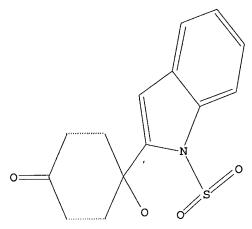
ring bonds:
1-2 1-6 2-3 3-4 4-5 5-6 9-10 9-13 10-11 11-12 11-14 12-13 12-17 14-15
15-16 16-17
exact/norm bonds:
1-2 1-6 2-3 2-7 3-4 4-5 5-6 5-8 9-10 9-13 10-11 12-13 13-18 18-19
18-20
exact bonds:
5-9
normalized bonds:
11-12 11-14 12-17 14-15 15-16 16-17

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 19:CLASS 20:CLASS

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100.0% PROCESSED 42 ITERATIONS 0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE** BATCH **COMPLETE** PROJECTED ITERATIONS: 452 TO 1228 PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> 11 full

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L3 14 SEA SSS FUL L1

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=> dup rem 14 PROCESSING COMPLETED FOR L4

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=> d ibib abs hitstr 1-4

ANSWER 1 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2006:565548 CAPLUS

DOCUMENT NUMBER: 145:224440

Antitumor quinols: Role of glutathione in modulating TITLE:

quinol-induced apoptosis and identification of

putative cellular protein targets

Chew, Eng-Hui; Matthews, Charles S.; Zhang, Jihong; AUTHOR (S):

McCarroll, Andrew J.; Hagen, Thilo; Stevens, Malcolm

F. G.; Westwell, Andrew D.; Bradshaw, Tracey D.

Centre for Biomolecular Sciences, School of Pharmacy, CORPORATE SOURCE:

University of Nottingham, Nottingham, UK

Biochemical and Biophysical Research Communications SOURCE:

(2006), 346(1), 242-251

CODEN: BBRCA9; ISSN: 0006-291X

PUBLISHER: Elsevier DOCUMENT TYPE: Journal LANGUAGE: English

Novel heteroarom. quinols 4-(benzothiazol-2-yl)-4-hydroxycyclohexa-2,5dienone (1) and 4-(1-benzenesulfonyl-1H-indol-2-yl)-4-hydroxycyclohexa-2,5dienone (2) are promising novel anticancer agents. They exhibit in vitro antiproliferative activity against colon, renal, and breast carcinoma cell lines as well as in vivo antitumor activity in colon, renal, and breast tumor xenografts. Elucidation of the mechanism of antitumor action of these compds. is of great importance. We show in this study that the compds. induced apoptosis as demonstrated by caspase 3 and PARP cleavage at doses causing G2/M cell cycle arrest. Glutathione was found to play an important role in modulating quinol-mediated cytotoxicity. In HCT 116 cells, treatment with 1 and 2 caused a 2- to 3-fold increase in the total glutathione content, suggestive of a glutathione-mediated antioxidant response. Indeed, buthionine sulfoximine (BSO)-induced glutathione

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CN

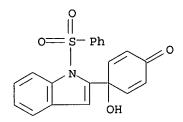
depleted cells were 6-10 times more sensitive to 1 and 2, while glutathione monoethyl ester supplementation decreased the antitumor potencies by 2-3 times. In further studies we determined other cellular proteins which bind to an immobilized quinol analog, and identified several proteins including β -tubulin, heat shock protein 60, and peroxiredoxin 1 as potential mol. targets of quinols that may contribute to their proapoptotic and antiproliferative effects. 719308-90-4

RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(antitumor quinols and role of glutathione in modulating quinol-induced apoptosis and identification of putative cellular protein targets)

RN 719308-90-4 CAPLUS

1H-Indole, 2-(1-hydroxy-4-oxo-2,5-cyclohexadien-1-yl)-1-(phenylsulfonyl)-(9CI) (CA INDEX NAME)



THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS REFERENCE COUNT: 25 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 2 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN L5

2005:375723 CAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 143:38034

Elucidation of thioredoxin as a molecular target for TITLE:

antitumor quinols

AUTHOR(S):

Bradshaw, Tracey D.; Matthews, Charles S.; Cookson, Jennifer; Chew, Eng-Hui; Shah, Manish; Bailey, Kevin; Monks, Anne; Harris, Erik; Westwell, Andrew D.; Wells, Geoffrey; Laughton, Charles A.; Stevens, Malcolm F. G.

Centre for Biomolecular Sciences, School of Pharmacy, CORPORATE SOURCE:

University of Nottingham, UK

Cancer Research (2005), 65(9), 3911-3919 SOURCE:

CODEN: CNREA8; ISSN: 0008-5472

American Association for Cancer Research PUBLISHER:

DOCUMENT TYPE: Journal LANGUAGE: English

Heteroarom. quinols 4-(benzothiazol-2-yl)-4-hydroxycyclohexa-2,5-dienone (1) and 4-(1-benzenesulfonyl-1H-indol-2-yl)-4-hydroxycyclohexa-2,5-dienone (2) exhibit potent and selective antitumor activity against colon, renal, and breast carcinoma cell lines in vitro (GI50 < 500 nmol/L). In vivo growth inhibition of renal, colon, and breast xenografts has been observed Profound G2-M cell cycle block accompanied down-regulation of cdk1 gene transcription was corroborated by decreased CDK1 protein expression following treatment of HCT 116 cells with growth inhibitory concns. of 1 or 2. The chemical structure of the quinol pharmacophore 4-(hydroxycyclohexa-2,5-dienone) suggested that these novel agents would readily react with nucleophiles in a double Michael (β -carbon) addition Indeed, COMPARE anal. within the National Cancer Institute database revealed a number of chemical related quinone derivs. that could potentially react with sulfur nucleophiles in a similar manner and suggested that

thioredoxin/thioredoxin reductase signal transduction could be a putative target. Mol. modeling predicted covalent irreversible binding between quinol analogs and cysteine residues 32 and 35 of thioredoxin, thereby inhibiting enzyme activity. Binding has been confirmed, via mass spectrometry, between reduced human thioredoxin and I. Microarray analyses of untreated HCT 116 cells and those exposed to either 1 (1 $\mu\text{mol/L})$ or 2 (500 nmol/L and 1 $\mu\text{mol/L})$ determined that of $\geq \! 10,000$ cancer-related genes, expression of thioredoxin reductase was up-regulated $> \! 3$ -fold. Furthermore, quinols 1 and 2 inhibited insulin reduction, catalyzed by thioredoxin/thioredoxin reductase signaling in a dose-dependent manner (IC50 < 6 $\mu\text{mol/L})$. Results are consistent with a mechanism of action of novel antitumor quinols involving inhibition of the small redox protein thioredoxin.

IT 719308-90-4

RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (elucidation of thioredoxin as mol. target for antitumor quinols)

RN 719308-90-4 CAPLUS

CN 1H-Indole, 2-(1-hydroxy-4-oxo-2,5-cyclohexadien-1-yl)-1-(phenylsulfonyl)-(9CI) (CA INDEX NAME)

REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:1142024 CAPLUS

DOCUMENT NUMBER: 142:219117

TITLE: Ouinols as Novel Therapeutic Agents. 2.

4-(1-Arylsulfonylindol-2-yl)-4-hydroxycyclohexa-2,5dien-1-ones and Related Agents as Potent and Selective

Antitumor Agents

AUTHOR(S): Berry, Jane M.; Bradshaw, Tracey D.; Fichtner, Iduna;

Ren, Ruobo; Schwalbe, Carl H.; Wells, Geoffrey; Chew, Eng-Hui; Stevens, Malcolm F. G.; Westwell, Andrew D.

CORPORATE SOURCE: Cancer Research U.K. Experimental Cancer Chemotherapy

Research Group, Centre for Biomolecular Sciences,

School of Pharmacy, University of Nottingham,

Nottingham, NG7 2RD, UK

SOURCE: Journal of Medicinal Chemistry (2005), 48(2), 639-644

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 142:219117

GI

A series of substituted 4-(1-arylsulfonylindol-2-yl)-4-hydroxycyclohexa-ΑB 2,5-dien-1-ones (indolylquinols) I (R = H, 5-OMe, 5-F, 6-F; R1 = H, 4-Me, 4-OMe, 2,4,6-triisopropyl) was synthesized on the basis of the discovery of lead compound I (R = R1 = H) and screened for antitumor activity. I was synthesized via the "one-pot" addition of lithiated (arylsulfonyl) indoles II to 4,4-dimethoxycyclohexa-2,5-dienone followed by deprotection under acidic conditions. Similar methodol. gave rise to the related naphtho-substituted quinols III (R1 = H, Me), 1H-indole- and benzimidazole-substituted quinols IV (X = CH, N). A number of compds. in this new series were found to possess in vitro human tumor cell line activity substantially more potent than the recently reported antitumor 4-substituted 4-hydroxycyclohexa-2,5-dien-1-ones with similar patterns of selectivity against colon, renal, and breast cell lines. I (R = 6-F, R1 = H), the most potent compound in the series in vitro, exhibited a mean GI50 = 16 nM and a mean LC50 = $2.24~\mu M$ in the NCI 60-cell-line screen, with LC50 activity in the HCT 116 human colon cancer cell line below 10 nM. The crystal structure of the unsubstituted indolylquinol I (R = R1 = H)exhibited two independent mols., both participating in intermol. hydrogen bonds from quinol OH to carbonyl O, but one OH group also interacts intramolecularly with a sulfonyl O atom. This interaction, which strengthens upon ab initio optimization, may influence the chemical environment of the bioactive quinol moiety. In vivo, significant antitumor activity was recorded (day 28) in mice bearing s.c. implanted MDA-MB-435 xenografts, following i.p. treatment of mice with I (R = R1 = H) at 50 mg/kg.

IT 719308-90-4P

RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (crystal structure; preparation and biol. activity of (arylsulfonylindolyl)hydroxycyclohexadienones as selective and potent antitumor agents)

RN 719308-90-4 CAPLUS

CN 1H-Indole, 2-(1-hydroxy-4-oxo-2,5-cyclohexadien-1-yl)-1-(phenylsulfonyl)-(9CI) (CA INDEX NAME)

RN 719308-92-6 CAPLUS
CN 1H-Indole, 5-fluoro-2-(1-hydroxy-4-oxo-2,5-cyclohexadien-1-yl)-1(phenylsulfonyl)- (9CI) (CA INDEX NAME)

RN 719308-93-7 CAPLUS
CN 1H-Indole, 2-(1-hydroxy-4-oxo-2,5-cyclohexadien-1-yl)-1-[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

RN 719308-94-8 CAPLUS

CN 1H-Indole, 2-(1-hydroxy-4-oxo-2,5-cyclohexadien-1-yl)-1-[(4-methoxyphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

RN 719308-95-9 CAPLUS

CN 1H-Indole, 1-[(4-fluorophenyl)sulfonyl]-2-(1-hydroxy-4-oxo-2,5-cyclohexadien-1-yl)- (9CI) (CA INDEX NAME)

RN 719308-96-0 CAPLUS

CN 1H-Indole, 2-(1-hydroxy-4-oxo-2,5-cyclohexadien-1-yl)-1-(2-naphthalenylsulfonyl)- (9CI) (CA INDEX NAME)

RN 719308-98-2 CAPLUS

CN 1H-Indole, 2-(1-hydroxy-4-oxo-2,5-cyclohexadien-1-yl)-1-[[2,4,6-tris(1-methylethyl)phenyl]sulfonyl]- (9CI) (CA INDEX NAME)

RN 719308-99-3 CAPLUS

CN 1H-Indole, 2-(1,4-dihydro-1-hydroxy-4-oxo-1-naphthalenyl)-1-(phenylsulfonyl)- (9CI) (CA INDEX NAME)

RN 719309-00-9 CAPLUS

CN 1H-Indole, 2-(1,4-dihydro-1-hydroxy-4-oxo-1-naphthalenyl)-1-[(4-

methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

RN 840474-95-5 CAPLUS

1H-Indole, 6-fluoro-2-(1-hydroxy-4-oxo-2,5-cyclohexadien-1-yl)-1-CN (phenylsulfonyl) - (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 4 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN

15

2004:550875 CAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER:

141:106370

TITLE:

Preparation of 4-[1-(sulfonyl)-1H-indol-2-yl]-4-

(hydroxy)-cyclohexa-2,5-dienone compounds and analogs

thereof as therapeutic agents

INVENTOR (S):

Stevens, Malcolm Francis Graham; Westwell, Andrew David; Poole, Tracey Dawn; Wells, Geoffrey; Berry,

Jane Marie

PATENT ASSIGNEE(S):

Cancer Research Technology Limited, UK

SOURCE:

PCT Int. Appl., 141 pp. CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.				KIND		DATE		APPLICATION NO.					DATE			
WO 2004056361				A1	20040708			WO 2002-GB5842					20021220			
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                                        20060511
PRIORITY APPLN. INFO.:
                                                      WO 2002-GB5842
                                                                                   20021220
                               MARPAT 141:106370
OTHER SOURCE(S):
GI
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This invention pertains to certain 4-(1-(sulfonyl)-1H-indol-2-yl)-4-AB (hydroxy)-cyclohexa-2,5-dienone compds., and analogs thereof, including compds. of the formula I [wherein Ar = 1-(sulfonyl)-1H-indol-2-yl; the bond marked α is a single bond or a double bond; the bond marked β is a single bond or a double bond; OR1 = OH, ether group (e.g., OMe) or acyloxy (i.e., reverse ester) group (e.g., -OC(O)Me); R2, R3, R5, R6 = H, monovalent monodentate substituent or a ring substituent which, together with an adjacent ring substituent, and together with the ring atoms to which these ring substituents are attached, form a fused ring; and pharmaceutically acceptable salts, esters, amides, solvates, hydrates, and protected forms thereof] which are, inter alia, antiproliferative agents, anticancer agents, and/or thioredoxin/thioredoxin reductase inhibitors. Syntheses of 11 representative compds. I are described. Thus, reacting 4,4-dimethoxycyclohexa-2,5-dienone (preparation given) with 1-benzenesulfonyl-1H-indole afforded 18% II 4-(1-benzenesulfonyl-1H-indol-2-yl)-4-hydroxycyclohexa-2,5-dienone which showed IC50 of 0.086 μM and 0.259 µM against HCT 116 and HT 29 growth (in vitro), resp. The present invention also pertains to pharmaceutical compns. comprising compds. I, and the use of such compds. I and compns., both in vitro and in vivo, for example, in the treatment of proliferative conditions, (e.g., cancer), and/or conditions mediated by thioredoxin/thioredoxin reductase. 719308-90-4P 719308-91-5P 719308-92-6P IT 719308-93-7P 719308-94-8P 719308-95-9P 719308-96-0P 719308-97-1P 719308-98-2P 719308-99-3P 719309-00-9P 719309-01-0P 719309-02-1P RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

RN 719308-91-5 CAPLUS
CN 1H-Indole, 2-(1-hydroxy-4-oxo-2,5-cyclohexadien-1-yl)-5-methoxy-1(phenylsulfonyl)- (9CI) (CA INDEX NAME)

RN 719308-92-6 CAPLUS
CN 1H-Indole, 5-fluoro-2-(1-hydroxy-4-oxo-2,5-cyclohexadien-1-yl)-1(phenylsulfonyl)- (9CI) (CA INDEX NAME)

RN 719308-93-7 CAPLUS
CN 1H-Indole, 2-(1-hydroxy-4-oxo-2,5-cyclohexadien-1-yl)-1-[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

RN 719308-94-8 CAPLUS

CN 1H-Indole, 2-(1-hydroxy-4-oxo-2,5-cyclohexadien-1-yl)-1-[(4-methoxyphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

RN 719308-95-9 CAPLUS

CN 1H-Indole, 1-[(4-fluorophenyl)sulfonyl]-2-(1-hydroxy-4-oxo-2,5-cyclohexadien-1-yl)- (9CI) (CA INDEX NAME)

RN 719308-96-0 CAPLUS

CN 1H-Indole, 2-(1-hydroxy-4-oxo-2,5-cyclohexadien-1-yl)-1-(2-naphthalenylsulfonyl)- (9CI) (CA INDEX NAME)

RN 719308-97-1 CAPLUS

CN 1H-Indole, 5-fluoro-2-(1-hydroxy-4-oxo-2,5-cyclohexadien-1-yl)-1-[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

RN 719308-98-2 CAPLUS

CN 1H-Indole, 2-(1-hydroxy-4-oxo-2,5-cyclohexadien-1-yl)-1-[[2,4,6-tris(1-methylethyl)phenyl]sulfonyl]- (9CI) (CA INDEX NAME)

RN 719308-99-3 CAPLUS

CN 1H-Indole, 2-(1,4-dihydro-1-hydroxy-4-oxo-1-naphthalenyl)-1-(phenylsulfonyl)- (9CI) (CA INDEX NAME)

RN 719309-00-9 CAPLUS
CN 1H-Indole, 2-(1,4-dihydro-1-hydroxy-4-oxo-1-naphthalenyl)-1-[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

RN 719309-01-0 CAPLUS
CN 1H-Indole, 1-[[5-(dimethylamino)-1-naphthalenyl]sulfonyl]-2-(1-hydroxy-4-oxo-2,5-cyclohexadien-1-yl)- (9CI) (CA INDEX NAME)

RN 719309-02-1 CAPLUS

CN 1H-Indole, 1-[[4-[3-(dimethylamino)propoxy]phenyl]sulfonyl]-2-(1-hydroxy-4-oxo-2,5-cyclohexadien-1-yl)- (9CI) (CA INDEX NAME)

4

REFERENCE COUNT:

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